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TITLE: # Exposure Estimates Using Urban Plume Dispersion and Traffic Microsimulation Models

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# EXPOSURE ESTIMATES USING URBAN PLUME DISPERSION AND TRAFFIC MICROSIMULATION MODELS

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## 1. INTRODUCTION

The goal of this research effort was to demonstrate a capability for analyzing emergency response issues resulting from accidental or meditated airborne toxic releases in an urban setting. In the first year of the program, we linked a system of fluid dynamics, plume dispersion, and vehicle transportation models developed at Los Alamos National Laboratory to study the dispersion of a plume in an urban setting and the resulting exposures to vehicle traffic. This research is part of a larger laboratory-directed research and development project for studying the relationships between urban infrastructure elements and natural systems.

## 2. METHOD

We performed numerical simulations of multiscale puff dispersion in an urban environment by linking together a microscale computational fluid dynamics (CFD) code and a prognostic mesoscale atmospheric transport and diffusion modeling system. With a passive gas source placed at street-level between two buildings, the relatively high resolution CFD code allowed us to model the diffusion of the puff within the urban canyon. After exiting the smaller CFD domain, the puff was injected into the larger mesoscale model domain. Here the puff transport and dispersion was followed for an hour over several kilometers. Independently, a microsimulation transportation model computed second-by-second trajectories of vehicles traveling in North Dallas. The computed ground-level concentration fields and vehicle trajectories were then used to estimate the exposure to the vehicles traveling through the plume (see fig. 1).

## 3. MODEL DESCRIPTIONS AND SET-UP

### a) Fluid dynamics codes

The mesoscale meteorological fields were computed by the HOTMAC (Higher-Order Turbulence Model for Atmospheric Circulation) model using nested grids of 2, 6, and 18 km horizontal resolution. HOTMAC utilizes a $1^1/_2$ order turbulence closure scheme, the hydrostatic approximation, and a terrain-following coordinate system (e.g., Yamada et al, 1989). The conservation equations for mass, momentum, heat, and moisture are solved numerically using the alternating direction implicit (ADI) finite difference scheme. The lower boundary conditions are defined by a surface energy balance and similarity theory. Sub-grid scale urban canopy effects are accounted for by building induced drag, turbulent kinetic energy (tke) production, and short and longwave radiation attentuation parameterizations (Brown and Williams, 1997).

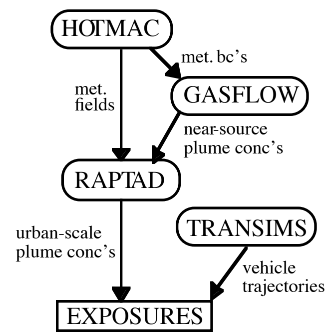


Figure 1. Flowchart showing the links between the mesoscale atmospheric model HOTMAC, the microscale fluid dynamics model GASFLOW, the Lagrangian dispersion model RAPTAD, and the TRANSIMS traffic simulation model.

The flow and concentration fields around two 2-d buildings were modeled using the GASFLOW CFD code (Travis et al., 1994) with an expanding rectilinear grid mesh ranging from 1 m near surfaces and expanding to 10 m at the domain top. GASFLOW solves the compressible Navier-Stokes equations and utilizes a $1^1/_2$ order turbulence closure scheme. Conservation equations are solved using the Implicit-Continuous Fluid-Eulerian Arbitrary- Lagrangian-Eulerian (ICEd-ALE) method and the van Leer advection scheme. Pressure is computed implicitly using the conjugate gradient solver. Concentration fields for a grid-cell-sized release are computed using GASFLOW's multiple species transport capability. HOTMAC-computed wind and turbulence fields and a neutral stability profile were used as inflow boundary conditions for the GASFLOW model.

The Eulerian concentration fields produced at the domain exit were then transformed into a Lagrangian puff framework for use in the HOTMAC/RAPTAD modeling system. Since the urban can-

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yon simulations were 2-d, we used the Briggs' urban $\sigma_y$ formulation for estimating the horizontal spread of the puff. The mesoscale concentration fields were then computed by RAPTAD (RAndom Particle Transport And Dispersion) using the mean and turbulent meteorological fields provided by HOTMAC. RAPTAD combines the attributes of random-walk and puff dispersion models. Pseudo-particles are transported with velocities that include a mean and turbulent component. The turbulent velocity is generated using the Monte-Carlo random-walk equation. Simultaneously, the particles grow with time following the random force theory of turbulent diffusion (e.g., Williams and Yamada, 1990).

Meteorological simulations centered over Dallas, Texas were carried out for forty-eight hours beginning at 19:00 lst on Oct. 22, 1996. Local airport rawinsonde measurements were used to initialize the HOTMAC model. At 07:00 lst on Oct. 23, a15-minute ground-level release was initiated near the intersection of the North Dallas Tollway and the LBJ Freeway. The dispersion simulations were carried out for several hours.

b) Traffic simulation code

The vehicle trajectories were computed by TRANSIMS (TRansportation ANalysis & SIMulation System), a microsimulation code that computes the movement of individual vehicles on a second-by-second basis using cellular automata techniques (Smith et al., 1995). Three of the primary modules of TRANSIMS are the household and commercial activity disaggregation, intermodal route planner, and travel microsimulation.

The first module creates a synthetic population that statistically matches the demographics of the real population based on census data. Using the synthetic information, travel activities and priorities for each household and traveler are produced.

The intermodal route planner produces trip plans for each traveler based on a demographically-defined travel cost decision model. The trip plans include the desired arrival and departure times at the origin and destination, the probable routes, and the travel mode choice.

The trip plans are passed to the travel microsimulation module which attempts to execute the plans for each traveler using cellular automata techniques. The roadway network is divided into cells of 7.5 length, roughly the size of a car. Each vehicle hops from cell to cell using simple rule sets for acceleration, deacceleration, lane changing, and intersection approaches (e.g., Rickert and

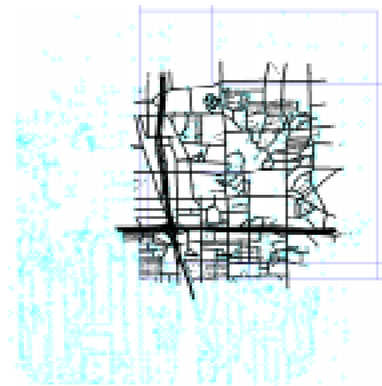

Figure 2. Major roadways impacted by the contaminant cloud. Diamonds represent network nodes and cover the entire active simulation region.

Nagel, 1997).

Over ten million trip plans were computed for travelers in the Dallas-Ft. Worth Metropolitan area for single occupancy vehicles. The detailed microsimulation was performed in a 5x5 mile area in North Dallas for over 250,000 vehicle trips (see fig. 2). Vehicle trajectories were computed on a second-by-second basis for a five hour period beginning at 5 am.

The simple rules of interaction among the vehicles on the microscale has been shown to result in macroscopic traffic patterns seen in common everyday traffic (e.g., Nagel and Rasmussen, 1994). Figure 3, a waterfall plot of vehicle position vs. time, depicts traffic shockwaves (congested regions) traveling backward in space. Figure 4 is a fundamental flow density diagram produced by TRANSIMS that is similar to those measured in real traffic.

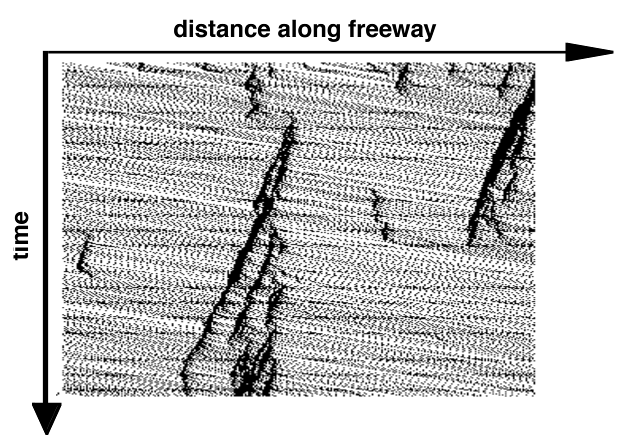


Figure 3. Waterfall plot showing vehicle locations as function of time produced by TRANSIMS. Vehicles traveling at constant speed produce a straight line with negative slope. The slope becomes smaller as the vehicle travels faster and becomes vertical as the vehicle velocity approaches zero. Traffic jams are apparent and congestion is shown to propagate upstream.

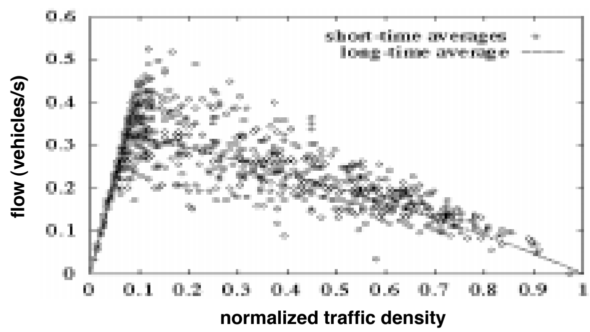


Figure 4. Fundamental flow density diagram showing a peak in flow at traffic density of 0.1. As traffic density becomes higher, flow drops off. Interestingly, the TRANSIMS model predicts a large variance at the location of maximum flow.

## 4. RESULTS AND DISCUSSION

### a) Meteorology and puff dispersion

Due to relatively smooth topography, the wind fields computed by the mesoscale model on the morning of Oct. 23 were southwesterly, in nearly the same direction as the large-scale synoptic flow. Because of HOTMAC urban-canopy parameterizations, however, the computed wind speed was appreciably smaller, the tke was larger, and the temperature was warmer over the Dallas-Ft. Worth area (fig.5).

Using the HOTMAC wind and turbulence fields as inflow B.C.'s, the GASFLOW simulation around two 2-d buildings reached steady state after 2 minutes (10,000 timesteps). At this time, the ground-level source located near the upstream edge of the downwind building was turned on. Figure 6 shows the computed steady-state concentration field. The pollutant was trapped between the buildings resulting in relatively high concentrations there. Some pollution was transported upstream due to recirculations and strong turbulent mixing that developed between the buildings and on the rooftop. As shown in Brown and Müller (1997), this enhanced vertical mixing dispersed the plume up to faster winds resulting in faster downwind transport of the plume as compared to a no-building case.

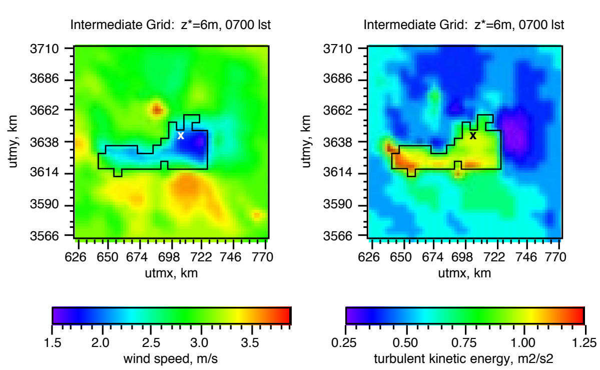


Figure 5. Magnitude of wind speed and tke computed by HOTMAC on the intermediate mesh. The outline and x denote the Dallas-Ft. Worth metropolitan area and the location of the urban canyon simulation, respectively.

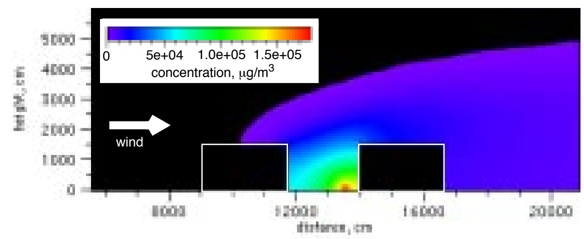


Figure 6. Concentration field computed by the GASFLOW model for a surface release in an urban canyon. Source strength = 100 g/s.

After the plume left the GASFLOW domain, it was injected into the HOTMAC/RAPTAD modeling domain. Figure 7 shows the temporal evolution of the ground-level concentration fields computed by RAPTAD over N. Dallas. Five minutes after release, the plume has traveled almost 2.5 km. After 15 minutes, the plume has traveled nearly 8 km and covers an area of approximately 15 km$^2$.

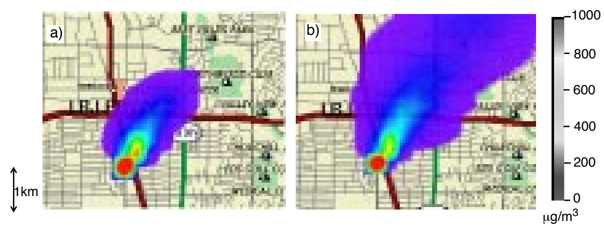


Figure 7. GLC fields computed by the GASFLOW/HOTMAC/RAPTAD modeling system a) 5 and b) 15 minutes after the start of the release.

### b) Vehicle exposure calculations

Vehicle trajectory and plume concentration data were used to compute exposures to over 36,000 vehicles traveling through the time-varying contaminant cloud according to the following:

$$\text{exposure} = \int_0^T \bar{C}(x, y, z{=}1.5\text{m}, t)\,dt$$

Hence, exposure represents what the vehicle drove through, and does not account for vehicle ventilation and driver breathing rates. The final location and exposure for each vehicle is shown in fig. 8. The contaminant is transported by the vehicles over a much larger area than the plume covers (fig. 9). Moreover, the final locations of vehicles with high exposure is not intuitively obvious.

## 5. CONCLUSIONS

By linking a microscale CFD code with a mesoscale atmospheric air quality modeling system, we modeled the transport and dispersion of a passive

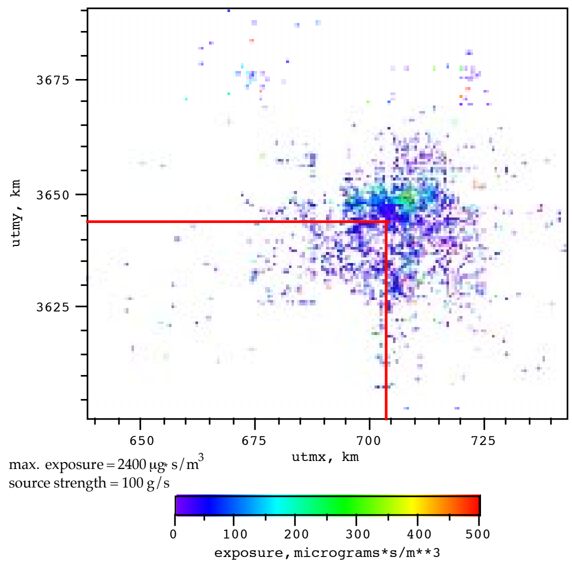


Figure 8. Vehicle exposure as function of final destination. Intersection of gray lines denote contaminant plume source location. The dimensions

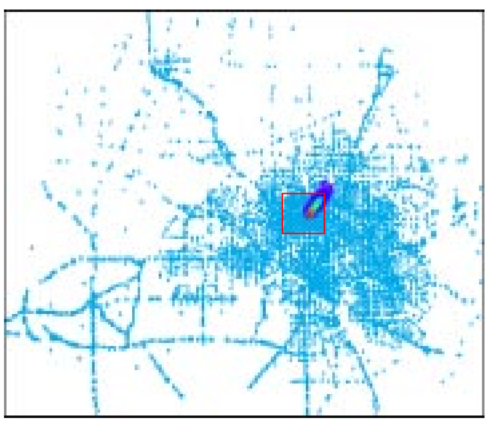

Figure 9. Node locations of the roadway network in the Dallas-Ft. Worth area. The spatial extent of the plume location 15 minutes after release is depicted. The gray box demarcates the region of active traffic simulation.

contaminant cloud through an urban canyon and onto the mesoscale topography in the vicinity of the Dallas-Ft. Worth area. Traffic simulations performed in N. Dallas by the TRANSIMS model were used in conjunction with the computed ground-level concentration fields to estimate exposures to the vehicles driving through the plume. In the event of an accidental spill or meditated release of a toxic agent in an urban environment, a modeling system like this shows promise for helping emergency response personnel determine impact zones, optimal routes for response teams, where casualties might occur, and how the agent is dispersed. The efforts of clean-up crews and medical teams could be enhanced as well with knowledge of the final location and levels of exposure.

This research effort was intended to demonstrate capabilities. The results should be interpreted with caution as a number of simplifications were made, including treating the urban canyon as 2-d, using empirical formulae for the horizontal plume spread, converting the concentration field from an Eulerian to a Lagrangian frame of reference, assuming a neutral stability inflow B.C. for the CFD simulation, accounting for single occupancy vehicle traffic only, and ignoring ventilation rates for vehicles. Future plume transport and dispersion research efforts will include performing 3-d urban canyon simulations, accounting for stability effects, and using a consistent dispersion model across computational domains. The TRANSIMS research team is expanding their capabilities as well, including efforts to perform city-wide simulations with full intermodal routing (cars, pedestrians, bikes, buses, light rail), using multi-resolution cellular automata, and calculating synthetic activities during the computation of the synthetic population.

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